

REACTING FLOW SIMULATIONS OF SUPERCRITICAL WATER OXIDATION OF PCB-CONTAMINATED TRANSFORMER OIL IN A PILOT PLANT REACTOR

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Abstract - The scale-up of a supercritical water oxidation process, based on recent advancements in kinetic aspects, reactor configuration and optimal operational conditions, depends on the research and development of simulation tools, which allow the designer not only to understand the complex multiphysics phenomena that describe the system, but also to optimize the operational parameters to attain the best profit for the process and guarantee its safe operation. Accordingly, this paper reports a multiphysics simulation with the CFD software Comsol Multiphysics 3.3 of a pilot plant reactor for the supercritical water oxidation of a heavily PCB-contaminated mineral transformer oil. The proposed model was based on available information for the kinetic aspects of the complex mixture and the optimal operational conditions obtained in a lab-scale continuous supercritical water oxidation unit. The pilot plant simulation results indicate that it is not feasible to scale-up directly the optimal operational conditions obtained in the isothermal lab-scale experiments, due to the excess heat released by the exothermic oxidation reactions that result in outlet temperatures higher than 600°C, even at reactor inlet temperatures as low as 400°C. Consequently, different alternatives such as decreasing organic flowrates or a new reactor set-up with multiple oxidant injections should be considered to guarantee a safe operation.

Keywords: SCWO; PCBs; Multiphysics simulation; Scale-up.

INTRODUCTION

Water is a supercritical fluid at temperatures and pressures above the critical point of water (374 °C and 22.13 MPa, respectively). Under these conditions, this substance has fascinating properties as a reaction medium (Shaw et al., 1991). For example, because many organic compounds and oxygen are readily soluble in supercritical water and form a single dense fluid phase, fast oxidation reactions can be carried out without mass transfer limitations. This has been used to effectively destroy highly stable organic pollutants with short residence times, as studies performed on the laboratory scale by several research groups have proven.

Supercritical water oxidation (SCWO) is thus considered to be one of the most promising technologies for treating toxic industrial wastes that cannot be handled by means of the conventional end-of-pipe technologies (Cocero et al., 2000, Veriansyah et al., 2005, Brunner, 2009).

In the supercritical water oxidation literature, most of the interest has been given to the destruction of the extremely toxic and possibly carcinogenic polychlorinated biphenyls (PCBs) (Hatakeda et al., 1999, Anitescu and Tavlarides, 2000, Weber et al., 2002, O'Brien et al., 2005, Marulanda and Bolaños, 2010), which were widely used in electrical transformers due to their insulating properties and resistance to thermal, chemical and biological

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degradation. SCWO of PCBs has been proposed as an alternative to incineration. The latter faces increasing public resentment since it is perceived to produce harmful byproducts such as polychlorinated dibenzofurans/dioxins (PCDFs/Ds), some of which are among the most toxic organic chemicals known (Greenpeace, 1998). Although destruction efficiencies greater than 99% have been reported for pure PCB congeners or PCB mixtures by means of SCWO, PCB contaminated mineral oils, resulting from the cross-contamination of fresh mineral oil with PCB from contaminated transformers during maintenance operations (UNEP, 2002), which account for most of the PCB stockpiles in South American countries, have been scarcely studied (Marulanda and Bolaños, 2010).

Despite its advantages over conventional end-of-pipe technologies, SCWO has not been fully developed on an industrial scale because of a lack of understanding of how some of the limitations of this technology can be avoided or controlled and many research efforts have been dedicated to address them. Significant advances have been made, for example, in areas related to corrosion control (Kritzer and Dinjus, 2001), proper handling of insoluble salts (Hodes et al., 2004), efficient reactor configurations (Kritzer and Dinjus, 2001), and the determination of the oxidation mechanisms and kinetics for a variety of chemical compounds (Crain et al., 1993).

The scaling up of supercritical water oxidation to a pilot plant level thus depends on the development of simulation tools that integrate the different advancements in reactor configurations and kinetic aspects to predict the performance of the proposed processes. In the recent literature, there are several approaches to the modeling and simulation of supercritical water oxidation processes through commercial computational fluid dynamics (CFD) simulation programs such as CFD-ACE (Zhou et al., 2000), STREAM (Masuda et al., 2006), Ansys CFX (Narayanan et al., 2008), NPHASE (Gallaway et al., 2008), COMSOL Multiphysics (Marulanda and Bolaños, 2008) and Fluent (Bermejo et al., 2010). These studies have focused on predicting the final conversion and temperature profile that can be achieved in an existing lab scale reactor and comparing the simulation with experimental results. While the simulation results agree well with the experimental lab scale data, simulation studies of a pilot plant operation, based on available information from previous research efforts, have not been carried out. Accordingly, this work reports a multiphysics simulation of the supercritical water oxidation of PCB contaminated mineral transformer oils in a pilot

plant reactor with the commercial software COMSOL Multiphysics 3.3, which uses a finite element method approach. The development of the pilot plant model was based on experimental results obtained in laboratory experiments with real PCB contaminated mineral oils and available information on the kinetic aspects of the complex mixture. This simulation is intended to provide insights into the technical feasibility of carrying out the destruction process in a mobile pilot plant as an alternative to incineration of PCB wastes, a technology that does not appear to be a viable treatment technology in South America in the near future.

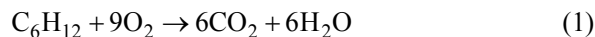
SCWO MODEL

The first step towards the development of a phenomenological model of a pilot plant reactor for the supercritical water oxidation of PCB wastes is the proper choice of the plant capacity and, therefore, the reactor volume. The latter depends on the organic contaminant and oxidant flow rates to be treated, which are based on available experimental information of reaction conditions such as temperature, oxidant excess, organic load and residence time under which the intended destruction efficiency of the organic matter and PCBs are to be attained. Marulanda (2009) studied the supercritical water oxidation of a heavily PCB contaminated mineral transformer oil in a continuous isothermal laboratory scale unit described in detail elsewhere. An experimental factorial design with temperature in the range of 500-550°C, oxidant excess in the range of 200%-400% and residence times in the range of 15-25 s and pressure of 241 bar was conducted in order to attain the optimal operational conditions. The dielectric oil contaminated with around 7200 ppm PCBs was obtained from an in-use electrical transformer. The contaminated oil was emulsified in water with the commercial emulsifier Arkopal® to reduce the viscosity and organic load content. The reaction progress under the experimental conditions of the proposed experimental design was followed by means of the disappearance of total organic carbon (TOC) and PCB congeners. Under the process conditions, the TOC and PCB concentration in the reactor inlet were 1268.4 mg/L (15.1 mol/m³ as cyclohexane) and 44.6 mmol/m³, respectively, at 539°C and 241 bar, 350% oxygen excess and 25 s of residence time. A 99.6% organic matter destruction, expressed as TOC, of the complex mixture of hydrocarbons and a PCB congeners concentration below the detection limit of the chromatographic

technique were obtained, which corresponds to a PCBs conversion of at least 99.999%.

Pilot Plant Capacity and Volume of the Reactor

50 kVA electrical distribution transformers are the most common in the electrical power sector, and it is generally accepted that 1 kVA corresponds to a content of 1 liter mineral oil. By defining an arbitrary feed of transformer mineral oil contaminated with PCBs to the reactor of 1 L/h at pump conditions of 25°C and 241 bar, conditions in which the processing of a distribution transformer could take up to two days, the corresponding hydrogen peroxide and dilution water flowrates can be calculated. Hydrogen peroxide solutions were used as the oxidant agent and the oxidant flow rate requirement to achieve a complete destruction of the organic matter was approached by assuming that the mineral oil is composed by pure cyclohexane, one of the major components of the hydrocarbons mixture, according to the oxidation reaction:



This approach proved to be effective for calculating the peroxide required to oxidize most of the organic matter when an oxygen excess in the range 100 to 250% over the stoichiometric amount was supplied, as required by the cyclohexane assumption (Marulanda, 2009). The total flow rate of aqueous 8 wt% hydrogen peroxide solution required to completely oxidize 1 L/h of mineral transformer oil, according to the available experimental results for the TOC in the reactor inlet, was calculated to be 467 L/h at the pump conditions of 25°C and 241 bar.

As indicated by Anitescu and Tavlarides (2000), the reactor volume V can be calculated from the residence time τ and the volumetric flow rate at the reactor inlet under supercritical conditions $v_{\text{SC},0}$ as follows:

$$\tau = V / v_{\text{SC},0} \quad (2)$$

The volumetric flow rate under supercritical conditions is calculated on the basis of a mass balance between the liquid phase at the pump outlet and the supercritical phase at the reactor entrance. The transport properties of the reactive mixture, density, viscosity, heat capacity and conductivity, were assumed to be those of supercritical water at the reaction conditions, since more than 95% of the reaction mixture is water. This approach has been

shown to be effective even for supercritical reactor simulations with computational fluids dynamics software (Marulanda and Bolaños, 2008).

Because the aim of this study is to model a pilot plant operation, commercial Swagelok 1.5 in (0.0381 m) external diameter, 0.02855 m internal diameter high pressure stainless steel tubing was specified for the construction of the reactor. The length of tubing required for 25 s of residence time according to Eq. (2) and an inlet temperature of 539°C is 66 m. Larger tubing diameters could not satisfy the mechanical strength safety requirement under the proposed reaction conditions and smaller diameters would result in an even longer reactor length. Although it is well known that stainless steel is not a sound choice for a chlorinated feed such as PCBs (Kritzer and Dinjus, 2001), from a process design, operation and economics perspective, it is easier to replace a tubing section of the whole reactor, usually the entrance section, that is affected by strong corrosion, than to build a reactor with expensive construction materials such as titanium alloys, or a mechanically complex flow configuration such as the transpiring wall reactor (Bermejo et al., 2010) or the floating type reactor (Lee et al., 2005). However, this consideration needs to be evaluated further by means of pilot plant studies and economic assessments.

Momentum Balance

With the flow rate under supercritical conditions and the reactor dimensions, the calculated Reynolds number is well over 180000, so that fully developed turbulent flow conditions prevail inside the reactor. COMSOL Multiphysics 3.3 uses the k - ϵ model to describe the turbulent flow. This model introduces two additional variables in the Navier-Stokes equation for laminar flow, the turbulent kinetic energy k and the dissipation of turbulent energy ϵ . Turbulence also creates problems in resolving the fluid dynamics near the walls because these regions include small and chaotic eddies, as well as boundary layer formation, so that the turbulent transport close to solid walls cannot be considered to be isotropic because the fluctuations resulting in turbulence vary greatly in magnitude and direction. In the k - ϵ model, an empirical relation between the value of the velocity and the wall friction, the logarithmic wall function, replaces the thin boundary layer and the no-slip boundary condition near the wall that is employed with the Navier-Stokes equations in laminar flow. Additional information on this model can be found elsewhere (Bird et al., 2002, COMSOL AB, 2006).

Mass Balance

The mass balance has a convective and a diffusive contribution as follows:

$$\frac{\partial c_i}{\partial t} + \nabla \cdot (-D_i \nabla c_i + c_i U) = R_i \quad (3)$$

here c_i is the concentration of reactant i in mol/m^3 , D_i is the diffusion coefficient in m^2/s , U is the superficial flow velocity in m/s and R_i is the reaction rate law. The first term in parentheses is the diffusion contribution and the second term is the convective contribution to the mass balance. When this balance is coupled to the k - ε turbulence model, the diffusivity is calculated as the ratio of turbulent viscosity, obtained from the momentum balance, to the density (COMSOL AB, 2006).

The reaction rate law for the destruction process of mineral transformer oil contaminated with PCBs must consider kinetic expressions for the mineral transformer oil, which is a complex hydrotreated light naphthenic distillate whose composition is unknown, and for the PCB congeners mixture, as both are indicative of the oxidation reaction's progress. Anitescu and coworkers (2000, 2002, 2004, 2005) studied the supercritical water oxidation of pure PCB congeners and of Aroclor 1248, a commercial PCB mixture widely used in electrical transformers, and determined a kinetic expression for the PCB disappearance rate by supercritical water oxidation using hydrogen peroxide as the oxidizing agent:

$$-r_{\text{PCBs}} = 10^{17.0 \pm 0.1} \text{s}^{-1} (\text{mol/L})^{-1} \exp\left(-\frac{(186 \pm 2 \text{kJ/mol})}{RT}\right) [\text{PCBs}]^{2.09 \pm 0.02} \quad (4)$$

The kinetic expression for the supercritical water oxidation of oily wastes such as mineral oils, which are important due to the high volume of generation in the industrial sector and high toxicity, has scarcely been studied. Most of the reported reaction rate laws in literature for supercritical water oxidation processes are for model compound, and only a few publications report kinetic expressions for complex residues in terms of the disappearance of the organic load of the mixture, either as chemical oxygen demand (COD) or total organic carbon (TOC), instead of the concentration of a model compound.

Sanchez-Oneto and coworkers (2007) studied the supercritical water oxidation of cutting oil wastes,

which are very similar in composition to the mineral transformer oils. They postulated that the organic matter destruction can be described by a first order rate law in terms of the disappearance of COD or TOC in two steps. The first step is a fast oxidation of most of the components of the organic mixture and the second step is a slow oxidation of intermediate byproducts that are more stable and that make it difficult to obtain a complete conversion to carbon dioxide and water. The slow oxidation step could be attributed to the formation of acetic acid, which has been identified as one of the most refractory intermediates in the oxidation of many complex organics in supercritical water oxidations. Because of the high stability of acetic acid, its oxidation is considered to be a critical, rate-limiting step in the total oxidation of organics to carbon dioxide and water (Krajnc and Levec, 1997). The refractory nature of acetic acid has therefore led many researchers to study its destruction in supercritical water (Savage and Smith, 1995, Lee, 1996).

Since the rate law expression for the disappearance of the organic load of PCB contaminated mineral transformer oils in supercritical water has not been reported, to the best of our knowledge, it is a good approach to use the kinetic expression for cutting oil wastes for the modeling of the tubular reactor of the mobile pilot plant treating PCBs contaminated mineral transformer oil. This approximation is supported by the fact that the composition of the oil is not constant, so that the optimization parameter is the disappearance of the organic load rather than the real composition of the oil, and the rate law for the cutting oil wastes should be valid for mineral oil if the composition of hydrocarbons is similar, as was indicated previously. The two step reaction rate law that was used in this work for the simulation of the supercritical water oxidation of mineral transformer oil is as follows (Sanchez-Oneto et al., 2007):

First step:

$$-r_{\text{TOC}} = 9.257 \times 10^3 \exp\left(-\frac{69100 \text{J/mol}}{RT}\right) [\text{TOC}] \quad (5)$$

Second step:

$$-r_{\text{TOC}} = 5.905 \times 10^5 \exp\left(-\frac{106900 \text{J/mol}}{RT}\right) [\text{TOC}] \quad (6)$$

According to Sanchez-Oneto and coworkers (2007) reported experimental results, the first step or

fast oxidation step describes the organic matter disappearance up to a conversion of 95% of the original TOC.

Figure 1 shows a comparison of the experimental disappearance of the total organic carbon of the mineral oil by supercritical water oxidation at 550°C, 241 bars and 350 % oxygen excess, and the values predicted by the proposed two-step rate law model of equations (5) and (6). Experimental values are available only for residence times longer than 15 s and these points agree reasonably well with the slow oxidation step (Equation (6)). However, no experimental data are available for times shorter than 15 s that would allow verification of the validity of the fast oxidation step (Equation (5)) of this two-steps rate law and, therefore, this model should be used with caution for modeling purposes.

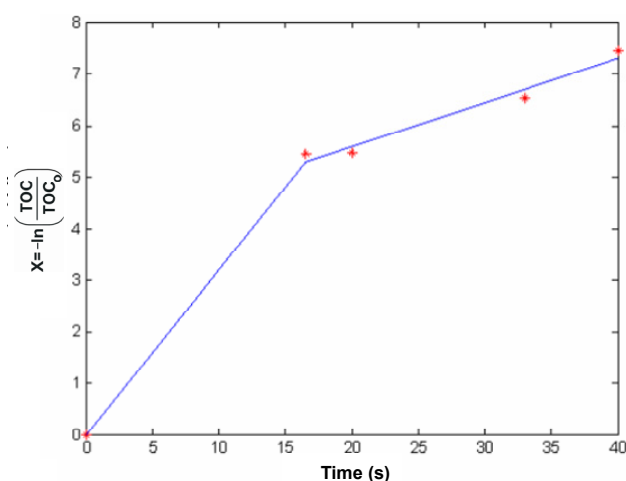


Figure 1: Experimental disappearance of total organic carbon of mineral oil by supercritical water oxidation with a two-step first order rate law (Marulanda, 2009)

Heat Balance

The general equation for the heat balance with heat transfer by conduction and convection is:

$$\rho C_p \frac{\partial T}{\partial t} + \nabla \cdot (-k \nabla T + \rho C_p T U) = Q \quad (7)$$

where C_p is the heat capacity at constant pressure in J/(kg.K), T is the temperature in K, k is the thermal conductivity in W/(m.K) and Q is the heat source or heat sink in W/m³. If the heat balance is coupled to the k - ϵ turbulence model, the thermal conductivity is automatically corrected to take into account the effect of intense mixing due to formation of eddies in

the reacting flow, so that the turbulence results in an effective thermal conductivity or turbulent conductivity (COMSOL AB, 2006). The heat source Q is the heat released by the simultaneous oxidation reactions of the transformer mineral oil and the PCBs and it can be calculated from the heat of the oxidation reaction, ΔH , in J/mol at the reaction temperature and the reaction rates, $(-r)$, in mol/(s.m³) of the two components, employing cyclohexane as a surrogate for the dielectric oil and biphenyl as a surrogate for PCBs:

$$Q = -r_{C_6H_{12}} \Delta H_{C_6H_{12}}(T) - r_{PCBs} \Delta H_{C_{12}H_{10}}(T) \quad (8)$$

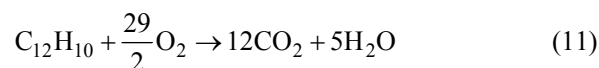
The heat released by the oxidation reaction under supercritical conditions can be estimated from the heat of formation under some standard condition, usually 25°C, and the overall change in the heat capacity per mole of oil reacted, assumed to be cyclohexane (See Eq. (1)), according to:

$$\Delta H(T) = \Delta H^\circ(25^\circ C) + \int_{25}^T \Delta C_p dT \quad (9)$$

The heat capacity in J/(mol.K) is frequently expressed as a function of temperature

$$C_{pi} = \alpha_i + \beta_i T + \gamma_i T^2 + \phi_i T^3 \quad (10)$$

Since the reaction heat is calculated per mole of cyclohexane, the rate law in terms of the total organic carbon disappearance in the mass and energy balances must also be expressed per mole of cyclohexane. Stoichiometrically, 1 mole of cyclohexane contains 6 moles of TOC. The reaction heat of PCB oxidation is approximated as the reaction heat for biphenyl oxidation. This assumption is supported by the reaction mechanism for PCB degradation in supercritical water suggested by Anitescu and Tavlarides (2002), where a rapid dechlorination takes place to give biphenyl, with subsequent biphenyl oxidation due to ring opening reactions:



Simulation Geometry and Boundary Conditions

Figure 2 shows a two dimensional radial and axial geometry model with angular and centerline symmetry for a tubular reactor with constant cross-

section. This geometry provides good simulation results without an excessive number of mesh elements and in short simulation times (COMSOL AB, 2006, Marulanda and Bolaños, 2008). Since the rate law for the disappearance of the total organic carbon is divided in two kinetic steps, a conditional expression was introduced into the model so that the first step rate law is used when TOC conversion is lower than 95% and the second step when TOC conversion is higher than or equal to 95%.

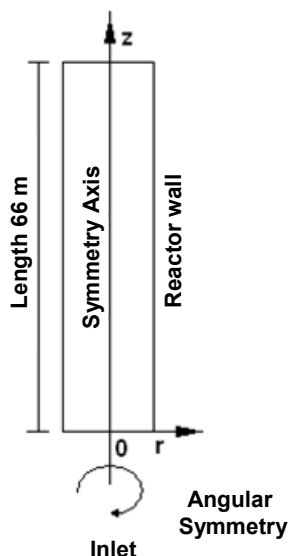


Figure 2: Two dimensional radial and axial geometry model with angular and centerline symmetry for a tubular reactor with constant cross-section.

Table 1 shows the selected boundary conditions for the momentum, heat and mass balances, according to the specified reactor geometry.

Table 1: Boundary conditions for momentum, heat and mass balances

Boundary condition	Momentum balance	Mass balance	Energy balance
Inlet	Inlet velocity	Inlet concentration	Inlet temperature
Outlet	Normal flow	Convective flux	Convection
Centerline (Symmetry axis)	Insulation Axial symmetry	Insulation Axial symmetry	Insulation Axial symmetry
Wall	Logarithmic wall (k-ε model)	Insulation	Adiabatic

RESULTS AND DISCUSSION

Figure 3 shows the simulated profiles of the reactor temperature and TOC conversion for the

proposed pilot plant tubular reactor with the reported optimal operational conditions obtained in the continuous lab scale experiments. The mesh size for the simulation consisted of around 13000 elements and the running time was 25 s on an AMD 3.01GHz processor with 2 GB ram memory. As observed in the profiles, piston flow conditions, which means that temperature and conversion are constant in the cross-section, are obtained along the reactor. The lack of radial dispersion in the profiles can be attributed to the fast heat and mass transfer in the highly turbulent flow. Although an unidimensional model could have been used to obtain similar results, as reported previously (Dutornié and Mercadier, 2004), the two-dimensional geometry is easy to model in Comsol and allows refinement of the proposed reactor set-up with, for example, multiple oxidant injections, as is further discussed in the results section.

Due to the heat released by the exothermic oxidation reactions of the contaminated oil and PCBs, the reactor outlet temperature increases rapidly in the reactor inlet up to 1031 K, which is unacceptable for a pilot plant operation. Different from the lab scale SCWO experiments, usually carried out at constant temperature in an isothermal sand bath reactor, the heat released by the oxidation speeds up the reaction rate, which at the same time releases more heat and increases the reaction temperature. Previous SCWO CFD simulation studies of lab scale experimental units have been carried out under heat sink reactor wall conditions (Marulanda and Bolaños, 2008), so that the heat released by the oxidation reactions is rapidly transferred to the sand bath and, as a result, almost isothermal conditions can be assumed. However, no such condition applies for the pilot plant operation. In fact, SCWO literature frequently points out the possibility of having autothermal conditions, which means that the reactor feed stream can be preheated with the heat released by the oxidation reaction so that no external heating is required under steady state operation, this being one of the main advantages of the process. In this regard, the reported optimal operational feed conditions for complete destruction obtained in lab scale experiments, in particular the temperature, are not the appropriate conditions under which to run a pilot plant operation. Whereas isothermal conditions prevail in lab scale experiments, the simulation results show, for feed conditions similar to those of the experiments, there is a temperature increase of around 200 K as a result of organic matter oxidation and adiabatic wall conditions.

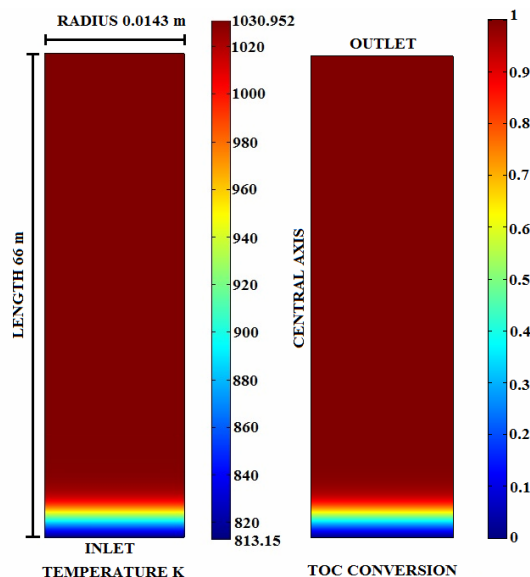


Figure 3: Simulated reactor temperature and TOC conversion profiles for the proposed pilot plant tubular reactor

Because SCWO process outlet temperatures higher than 1000 K are technically unfeasible due to the mechanical strength limitation of the reactor construction materials, a lower feed inlet temperature should be used to avoid unsafe operation temperature conditions while keeping the organic load and PCBs destruction targets the same as those of the experiments. A lower feed temperature in comparison to those usually reported in lab scale SCWO experiments also contributes to improving the perception of the technical feasibility of the process, since the preheating energy consumption could be drastically reduced, not to mention the possibility of carrying out an autothermal operation. Accordingly,

parametric temperature simulation studies were carried out in order to assess an appropriate feed temperature that guarantees a technically feasible operation; this corresponds to a reactor outlet temperature lower than 900 K for organic matter and PCBs destruction that is practically 100%. Figure 4 shows the temperature along the reactor central axis for different reactor inlet temperatures, Figure 5 shows the TOC conversion and Figure 6 the PCBs conversion variations with inlet temperature. As shown in Figure 3, plug flow conditions prevail and the central temperature should be practically the same as that near the reactor wall and hence no integration over the reactor cross-section is required.

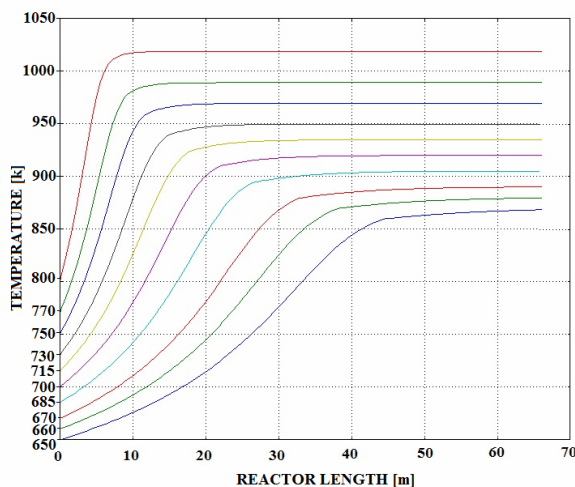


Figure 4: Temperature along the reactor central axis for different reactor inlet temperatures

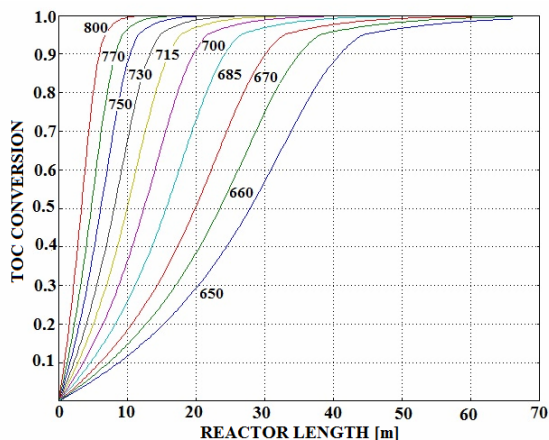


Figure 5: TOC conversion variation with inlet temperature along the reactor

As shown in Figure 4, reactor outlet temperatures higher than 900 K (627°C) are obtained for inlet temperatures higher than 685 K (412°C). Temperatures higher than 600°C are not appropriate for pilot plant operation. Figure 6 shows that a PCBs conversion near 100% is obtained for an inlet temperature of 650 K; however, TOC conversion (see Figure 5) is not complete. Due to the possibility of the formation of chlorinated byproducts with dielectric oil oxidation intermediates, a total organic oxidation or TOC destruction higher than 99% should be met. Figure 5 shows that, for a 660 K inlet temperature, a TOC conversion near 100% is obtained. 660 K results in an outlet temperature of 880 K (607°C) still too high for a safe pilot plant operation.

The results indicate that operation of a pilot plant consisting of a tubular reactor with adiabatic conditions is not feasible due to the excess heat released by the oxidation reactions, even at inlet temperatures near 400°C. In order to attain safe operational conditions, the heat released could be reduced by decreasing the inlet organic flowrate or the TOC concentration or by providing reactor cooling. However, these measures work against the potential profitability of the process. Portela and coworkers (2007) developed a multi-injection oxidant reactor set-up that distributes the quantity of oxygen along the reactor in order to improve the thermal control of the process, avoiding hot spots in the reactor. Because SCWO studies of model compounds are usually carried out in conditions of excess oxygen, the rate law expressions do not account for oxygen concentration and, therefore, do not allow assessment of the effect of multiple oxygen

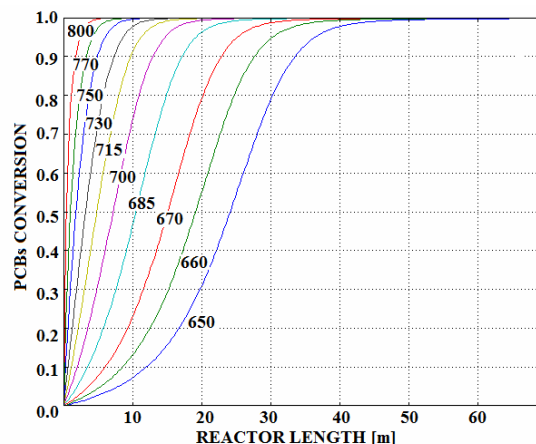


Figure 6: PCBs conversion variation with inlet temperature along the reactor

injections along the reactor. A reactor model with multiple oxidant injections could be used to attain a more feasible operation for the treatment of heavily PCB contaminated transformer mineral oils. However, the rate law expressions must include the oxygen concentration dependence. This study can easily be performed by means of Comsol Multiphysics and will be the subject of a different publication.

CONCLUSIONS

SCWO scale up to the pilot plant level requires the development of simulation tools that allow integrating the different advancements in reactor configurations, kinetic aspects and optimal operational conditions, in order to reduce the amount of experimental work and attain a more reliable operation. In this work, the simulation of the SCWO of a PCB contaminated transformer mineral oil in a pilot plant, based on optimal operational conditions determined in a lab scale study, was carried out. Simulations showed that the proposed pilot plant operation was not feasible due to the high temperature that results from the exothermic oxidation reactions of the organic matter, even with inlet temperatures near 400°C. For the purpose of decreasing the reaction temperature and attaining a safe operation without decreasing the organic flow rates or providing external cooling, the oxidant could be fed through multiple injection ports along the reactor, as has been suggested in the literature for a pilot plant oxidation of an organic waste. However, this would require a kinetic expression that accounts

explicitly for the oxygen effect, which is not usually available because rate laws are determined via experiments at high excess oxygen where its effect can be neglected. This points to the necessity of carrying out lab scale experiments in which the kinetic expressions obtained can be used for scale up purposes, since, as was shown in this work, the optimal operational conditions are not necessarily those under which pilot plant operation is feasible.

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